P 9 Sensitivity and control of evolutions with rate-independent elements (M. Brokate, K. Fellner, K. Kunisch, M. Ulbrich) $\rightarrow$ NS, IS

This project is concerned with optimal control of evolution problems with rate-independent elements. Its focus lies on the analysis and numerical treatment of the controlled evolution system, based on generalized differentiability properties of the associated control-to-state mapping. Problems for ordinary differential equations as well as for reaction-diffusion systems are treated.

State of the art. Optimal control problems for reaction-diffusion equations were considered in [12] and later in e.g. [13, 2]. Recent papers concerning numerics of such control problems are [22, 20]. Feedback control for reaction-diffusion equations was considered in [7, 11]; in [7], a hysteresis operator appears in the boundary condition. Papers [15, 14, 16] treat reaction-diffusion equations with distributed hysteresis of switching type.

The theory of systems of reaction-diffusion equations is significantly harder than in the scalar case, because comparison principles and, specifically, the maximum principle are no longer available. Thus, for many general nonlinear reaction-diffusion systems, global-in-time existence of (weak or classical) solutions constitutes an open problem, in particular in the physical space 3D. Promising recent advances were made by applying various duality methods in particular in connection with using entropy variables, (see e.g. the survey [23] and [10, 6]).

Concerning the numerical solution of the optimality system for a controlled evolution with smooth dynamics, semismooth Newton methods usually come into play when the optimality system is not smooth, due to the presence of constraints or of a nonsmooth cost functional. This is now well established; see e.g. the papers [18, 8, 9] which also illustrate that often a regularization is required. However, the presence of rate-independent elements in the dynamics introduces an additional source of nonsmoothness. Discretization of rate-independent evolutions (with or without a control context) has been discussed in [25, 19, 21, 24, 1]. Semismooth Newton methods have been used in plasticity for solving the fully discretized problem [17]. In order to consider semismooth Newton methods for a control problem in a function space setting, however, the rate-independent part needs to possess certain weak differentiability properties. Such results are now emerging, apparently for the first time, see [4]. In the context of HJB equations, there are results concerning the semismoothness of certain maximum operators, the maximum being taken over a compact metric space (instead of a finite set), see [26].

First thesis project: *Control of reaction-diffusion systems with hysteresis* to be supervised by Martin Brokate. This thesis project is devoted to *Control of reaction-diffusion systems with hysteresis*. The model dynamics is given by the following prototypical system of reaction-diffusion equations for concentrations y_1 and y_2,

$$\partial_t y_1 - D_1 \Delta y_1 = f_1(y_1, y_2, w)\,, \tag{1}$$
$$\partial_t y_2 - D_2 \Delta y_2 = f_2(y_1, y_2, w)\,, \tag{2}$$

in some cylindrical domain $\Omega_T = \Omega \times (0,T)$ plus initial and (e.g. non-flux) boundary conditions, which is coupled to the equation

$$w(t) = \mathcal{W}[S(y_1, y_2)](t) \tag{3}$$

where $\mathcal{W}$ is a rate-independent causal (= hysteresis) operator and S is an operator which maps (y_1, y_2) to a function from $[0,T] \to \mathbb{R}$. A particular case is given by

$$S(y_1, y_2)(t) = \int_\Omega y_1(x,t) + y_2(x,t)\, dx\,, \tag{4}$$

so $S(y_1, y_2)$ denotes the total mass arising from the concentrations y_1 and y_2. Here, the hysteresis operator represents a buffer mechanism which modulates $w(t)$ in dependence on the total mass. An applicational background for such models stems from large reaction-diffusion systems in biology or chemistry, where the dynamics in y_1 and y_2 is complemented by a (fast) buffer dynamics of other concentrations, lumped together and heuristically or asymptotically approximated by the rate-independent operator $(y_1, y_2) \mapsto \mathcal{W}[S(y_1, y_2)]$.

The thesis project will focus on an associated optimal control problem. Namely, one minimizes

$$J(y,u) = \int_\Omega \sum_{i=1}^{2} (y_i(x,T) - y_{i,d}(x,T))^2\, dx + \int_0^T \int_\Omega u(x,t)^2\, dx\, dt \tag{5}$$

subject to the dynamics

$$\partial_t y_1 - D_1 \Delta y_1 = f_1(y_1, y_2, w) + u\,, \tag{6}$$

$$\partial_t y_2 - D_2 \Delta y_2 = f_2(y_1, y_2, w)\,, \tag{7}$$

where u is the control, coupled to the rate-independent part given by (3) and (4), and complemented by initial and boundary conditions.

The main goal is to derive the first order optimality system. The essential difficulty is the nonsmoothness of the operator $\mathcal{W}$. First, one derives the wellposedness of the dynamical system for a given control, by extending the results of [27] concerning parabolic equations with hysteresis. Next, the differentiability of the control-to-state mapping will be investigated, based on the corresponding results for the hysteresis operator in [4]. This will then lead to the derivation of first order optimality conditions. Technical challenges, however, will arise since the analytical treatment of the system (6), (7) is more difficult than the corresponding single equation, and since generalized derivatives of $\mathcal{W}$ require certain function space settings. Here, we hope to extend current duality- and entropy methods in order to overcome these difficulties, see e.g. [10].

Further topics – first project. Extending the tasks related to (1) – (4), there are several natural generalizations. First, larger reaction-diffusion systems of three and more equations will lead to even greater analytical challenges. Secondly, one could consider estimates for the large time behavior, in particular results on the convergence to an equilibrium state. Moreover, it would be highly interesting to study how a rate-independent operator like $\mathcal{W}[S(\cdot,\cdot)]$ could be derived in a singular (e.g. a fast-reaction) limit from larger reaction-diffusion systems. Finally, it would be of interest to consider hysteresis operators as part of the boundary conditions.

One may also consider (1) – (4) as a feedback control problem with parameters of $\mathcal{W}$ to be designed.

Second thesis project: *Semismooth Newton methods for evolutions with a rate independent part* to be supervised by Martin Brokate. This thesis project is devoted to *Semismooth Newton methods for evolutions with a rate-independent part*. The model problem for the overall evolution is given by an ODE system coupled with a rate-independent operator $\mathcal{W}$,

$$y' = f(y, w) + Bu \,, \quad w = \mathcal{W}[y] \,, \tag{8}$$

where u is the control and B is a matrix of appropriate dimension. The first task is to establish the semismoothness of the operator $\mathcal{W}$ in suitable function spaces, based on and extending the results from [4]. Preliminary computations show that in a special situation this is indeed the case; the generalized derivative needed for semismoothness (the Newton derivative) involves a suitable family of measures. As a second step, the semismoothness of the control-to-state mapping $u \mapsto (y, w)$ has to be established. For both steps above, one has to choose suitable norms (which may turn out to be different ones) in the domain and the range of the generalized derivative of $\mathcal{W}$. Next, an associated optimal control problem will be considered. Namely, one wants to

$$\text{minimize} \quad J(y, w, u) = \int_0^T L(y, w, u)\, dt + L_T(y(T)) \tag{9}$$

subject to (8) on some interval $[0, T]$, augmented by an initial condition $y(0) = y_0$, and a control constraint $u(t) \in U$.

Based on the generalized derivative of the control-to-state mapping, the first order optimality system will be derived; this will improve the result in [3].

Then, a numerical algorithm will be developed in order to solve the optimality system by the semismooth Newton method. First, the algorithm is constructed in a suitable function space. The goal is to transform the optimality system into the form

$$F = 0 \,, \tag{10}$$

where F is a Newton-differentiable mapping between suitable function spaces. By the foregoing, the state equation already has the required properties. For the adjoint equation, a regularization will have to be employed, since the adjoint equation will include the generalized derivative of $\mathcal{W}$ which is not expected to be semismooth. The treatment of the control constraint will possibly also use a regularization step, see e.g. [8]. Finally, one will prove that the inverses DF^{-1} are uniformly bounded, so the general convergence result for the semismooth Newton method applies.

For actual numerical computations, a fully discrete method is needed. This will involve the discretization of the Newton derivative of $\mathcal{W}$ and its coupling with the integration method. Numerical experiments will be conducted in order to study the behavior of the algorithm and to improve the understanding of the control problem.

Further topics – second project. In addition to (8), terminal conditions or state constraints can be included. This raises questions of controllability and of multiplier regularity, respectively, which have to be addressed in view of the rate-independent operator $\mathcal{W}$.

One may also replace the ODE in (8) with a semilinear parabolic equation. Once the optimality conditions for the corresponding optimal control problem are obtained, which is work in progress, a semismooth Newton method can be developed along the lines described above.

In a next step, one should consider an ODE problem of the form

$$y' + (g(w))' = f(t, y, w) + Bu \,, \quad w = \mathcal{W}[y] \,.$$

In order to obtain semismoothness of the associated control-to-state mapping, properties of inverses $(I + \mathcal{W})^{-1}$ of rate-independent operators play a role, see e.g. [5].

There is also the question whether it is possible to derive generalized second order conditions for the ODE control problem. Currently, this problem appears to be completely open.

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